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Mathematics

Extended Watson integrals for the cubic lattices

(elliptic integral/trigonometric polynomial)

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ABSTRACT The known exact expressions for extended Watson integrals relating to various cubic and modified cubic lattices are summarized. A new closed form expression for Watson's result on the simple cubic lattice is given in terms of gamma functions.

Nearly 40 years ago, G. N. Watson (1) evaluated the three triple integrals

$$I_1(z) = \frac{1}{\pi^3}\int\int_0^\pi\int \frac{du\,dv\,dw}{z - \cos u \cos v \cos w}, \quad z = 1$$

$$I_2(z) = \frac{1}{\pi^3}\int\int_0^\pi\int \times \frac{du\,dv\,dw}{z - \cos u \cos v - \cos v \cos w - \cos w \cos u}, \quad z = 3 \quad [1]$$

$$I_3(z) = \frac{1}{\pi^3}\int\int_0^\pi\int \frac{du\,dv\,dw}{z - \cos u - \cos v - \cos w}, \quad z = 3$$

which had been passed on to him via Kramers, Fowler, and Hardy. These integrals arise in the study of various physical phenomena relating to transport on body centered, face centered, and simple cubic lattices, respectively. Since that time, these integrals have been studied extensively for arbitrary values of z. The first purpose of this note is to present, in one place, analytic expressions for these integrals and related ones, in terms of the complete elliptic integral of the first kind. Watson was able to express $I_1(1)$ and $I_2(3)$ in terms of the gamma function of simple rational arguments, but such an expression has been missing for $I_3(3)$; the second purpose of this note is to supply one. This work grew out of the authors' independent investigations of when the complete elliptic integral of the first kind is reducible to the gamma function, which will be presented elsewhere.

The basic results are:

$$I_1(z) = (4/z\pi^2)K^2(k) \quad [2]$$

in which

$$k = 2^{-1/2}[1 - (1 - z^2)^{1/2}]^{1/2}, \quad z \geq 1 \quad [2a]$$

which is due to Maradudin *et al.* (2);

$$I_2(z) = (4/\pi^2)(z + 1)^{-1}K(k_+)K(k_-) \quad [3]$$

in which

$$k_\pm^2 = (z + 1)^{-2}\left[\frac{1}{16}\{(z + 1)^{1/2} - (z - 3)^{1/2}\}^4 + \{(z + 1)^{1/2} \pm z^{1/2}\}\right], \quad z \geq 3 \quad [3a]$$

derived by Iwata (3); and

$$I_3(z) = (8/\pi^2 z)\left\{\frac{(\xi + 1)(\xi + 4)}{\xi^2 + 8\xi + 8 + 4(2 + \xi)(\xi + 1)^{1/2}}\right\}^{1/2} \times K(k_+)K(k_-) \quad [4]$$

in which

$$k_\pm^2 = \frac{\xi[(\xi + 1)^{1/2} \pm (\xi + 4)^{1/2}] - 2[1 - (\xi + 1)^{1/2}]}{\xi[(\xi + 1)^{1/2} \pm (\xi + 4)^{1/2}] + 2[1 + (\xi + 1)^{1/2}]} \quad [4a]$$

and

$$\xi = \frac{z^2 + 3 - [(z^2 - 9)(z^2 - 1)]^{1/2}}{z^2 - 3 + [(z^2 - 9)(z^2 - 1)]^{1/2}}, \quad z \geq 3 \quad [4b]$$

first derived by Joyce (4)‡. The indicated ranges for z are easily extended by analytic continuation.

From Eq. **2**–Eq. **4b** we easily obtain Watson's results

$$I_1(1) = \frac{4}{\pi^2}K^2(2^{-1/2})$$

$$I_2(3) = \frac{1}{\pi^2}K\left(\frac{\sqrt{2 + \sqrt{3}}}{2}\right)K\left(\frac{\sqrt{2 - \sqrt{3}}}{2}\right) \quad [5]$$

$$I_3(3) = (8/3\pi^2)\,[10(17 - 12\sqrt{2})]^{1/2}K[(2 - \sqrt{3}) \times (\sqrt{3} + \sqrt{2})]K[(2 - \sqrt{3})(\sqrt{3} - \sqrt{2})].$$

For completeness we list three related formulas pertaining to modified cubic lattices:

$$\frac{1}{\pi^3}\int\int_0^\pi\int \frac{du\,dv\,dw}{(2 + \alpha^2) - \cos u - \cos v - \alpha^2 \cos w} = (4/\alpha\pi^2)[(\gamma + 1)^{1/2} - (\gamma - 1)^{1/2}] \times K(k_+)K(k_-) \quad [6]$$

in which

$$k_\pm = \frac{1}{2}[(\gamma - 1)^{1/2} \pm (\gamma - 3)^{1/2}] \times [(\gamma + 1)^{1/2} - (\gamma - 1)^{1/2}] \quad [6a]$$

and

$$\gamma = (4\alpha^{-2} + 3) \quad [6b]$$

given by Montroll (cf. ref. 2);

$$\frac{1}{\pi^3}\int\int_0^\pi\int \times \frac{du\,dv\,dw}{(2 + \alpha^2) - z(\cos u \cos v + \cos v \cos w + \alpha^2 \cos w \cos u)} = (4/\pi^2)\frac{(2 + \alpha^2)^2}{(2 + \alpha^2 + \alpha^2 z)}K(k_+)K(k_-) \quad [7]$$

in which

$$k_\pm^2 = \frac{1}{2} \pm \frac{2z\alpha(2 + \alpha^2)^{1/2}(\alpha^4 + 2\alpha^2 + z)^{1/2}}{(2 + \alpha^2 + \alpha^2 z)^2} \quad [7a]$$

$$-\frac{1}{2}\frac{(2 + \alpha^2)^{1/2}(2 + \alpha^2 - \alpha^2 z)[(2 + \alpha^2) + (2 - \alpha^2)z]^{1/2}}{(2 + \alpha^2 + \alpha^2 z)^2} \times (1 - z)^{1/2} \quad [7b]$$

‡ This derivation, which led to an expression equivalent to Eq. 4, used Heun functions. The result given in Eq. 4 was subsequently obtained by Glasser using Lauricella functions (see ref. 11).

due to Joyce (5); and

$$\frac{1}{\pi^3}\int\int_0^\pi\int \frac{dudvdw}{z-[\cos u\cos v\cos w+(\cos u\cos v+\cos v\cos w+\cos w\cos u)+(\cos u+\cos v+\cos w)]} = \frac{32}{\pi^2(z+1)}K^2(k) \quad [8a]$$

in which

$$k^2 = \frac{1}{2}\left[1-\left(\frac{z-1}{z+1}\right)^{1/2}\right] \quad [8b]$$

due to Glasser (6).

The problem of when

$$K(k) = \int_0^{\pi/2}\frac{d\phi}{\sqrt{1-k^2\sin^2\phi}}$$

can be expressed in terms of gamma functions of rational arguments apparently goes back to Abel (7). Our investigations, which extend results of Selberg and Chowla (8), Weil (9), and Kummer (10), indicate this should be possible when $r = (K'/K)^2$, in which $K' = K[(1-k^2)^{1/2}]$, is rational. The three cases in Eq. **5** correspond to $r = 1$, 3, and 6, respectively, for which values we obtain

$$I_1(1) = \Gamma^4(1/4)/4\pi^3$$

$$I_2(3) = 2^{-14/3}(3/\pi^4)\Gamma^6(1/3)$$

$$I_3(3) = (4\sqrt{6}/\pi^2)\Gamma(1/24)\Gamma(5/24)\Gamma(7/24)\Gamma(11/24)$$

We wish to conclude with the following conjecture: let ϕ denote any ternary trigonometric polynomial in u, v, w. Then,

$$\frac{1}{\pi^3}\int\int_0^\pi\int\frac{dudvdw}{z-\phi} = AK(k_1)K(k_2)$$

in which A, k_1, k_2 are algebraic functions of z. This has been verified explicitly (11) in more than 20 cases besides those summarized here.

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